=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:13:11 ON 29 DEC 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 DEC 2005 HIGHEST RN 870751-96-5
DICTIONARY FILE UPDATES: 28 DEC 2005 HIGHEST RN 870751-96-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

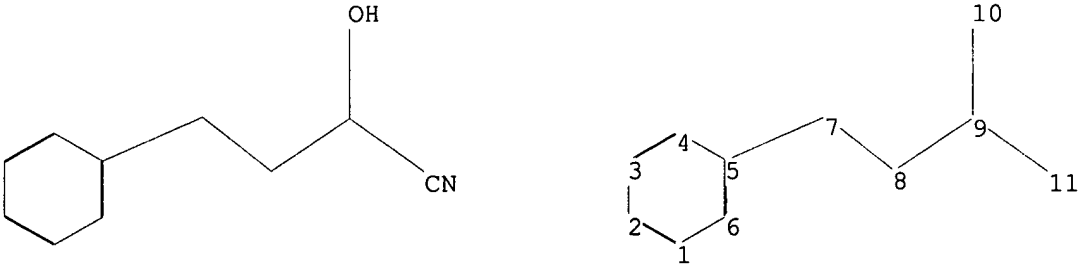
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10719660b.str



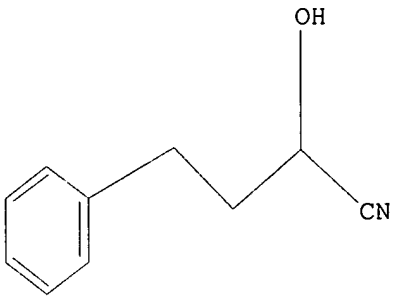
chain nodes :
7 8 9 10 11
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 7-8 8-9 9-10 9-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :

9-10
exact bonds :
5-7 7-8 8-9 9-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:13:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   108 TO ITERATE

100.0% PROCESSED   108 ITERATIONS   8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 1537 TO   2783
PROJECTED ANSWERS: 8 TO   329

L2   8 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:13:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2015 TO ITERATE

100.0% PROCESSED   2015 ITERATIONS   152 ANSWERS
SEARCH TIME: 00.00.01

L3   152 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   161.33   161.54

FILE 'CAPLUS' ENTERED AT 15:13:27 ON 29 DEC 2005
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FILE COVERS 1907 - 29 Dec 2005 VOL 144 ISS 1
FILE LAST UPDATED: 28 Dec 2005 (20051228/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 205 L3

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	161.99

FILE 'REGISTRY' ENTERED AT 15:13:39 ON 29 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 28 DEC 2005 HIGHEST RN 870751-96-5
DICTIONARY FILE UPDATES: 28 DEC 2005 HIGHEST RN 870751-96-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************
```

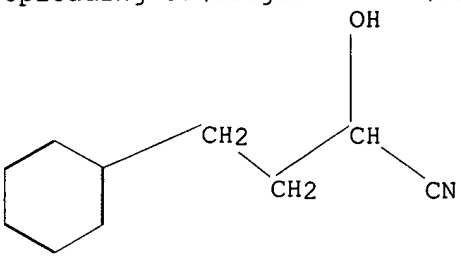
Structure search iteration limits have been increased. See HELP SLIMITS for details.

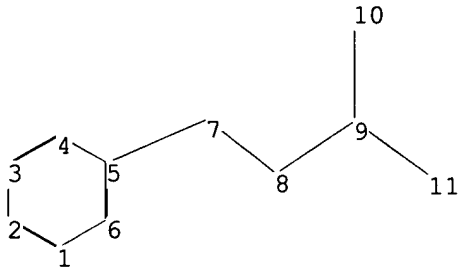
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of

experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10719660c.str



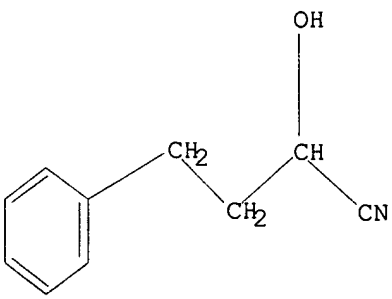


chain nodes :
7 8 9 10 11
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 7-8 8-9 9-10 9-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
9-10
exact bonds :
5-7 7-8 8-9 9-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l5
SAMPLE SEARCH INITIATED 15:14:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      108 TO ITERATE

100.0% PROCESSED      108 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1537 TO     2783
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l5 full
FULL SEARCH INITIATED 15:14:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2015 TO ITERATE

100.0% PROCESSED     2015 ITERATIONS                                  7 ANSWERS
SEARCH TIME: 00.00.01

L7            7 SEA SSS FUL L5

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     161.33     323.32

FILE 'CAPLUS' ENTERED AT 15:14:19 ON 29 DEC 2005
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FILE COVERS 1907 - 29 Dec 2005  VOL 144 ISS 1
FILE LAST UPDATED: 28 Dec 2005  (20051228/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l7
L8            76 L7

=> s l7/p
L9            58 L7/P

=> s l9 and ester
        570950 ESTER
        425597 ESTERS
        797525 ESTER
                  (ESTER OR ESTERS)
L10            9 L9 AND ESTER
```

=> d ibib abs hitstr tot

L10 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:509058 CAPLUS
DOCUMENT NUMBER: 139:213884
TITLE: Cyanobenzoylation and Hydrocyanation of Aldehydes with
Benzoyl Cyanide Using No Catalyst
AUTHOR(S): Watahiki, Tsutomu; Ohba, Sayoko; Oriyama, Takeshi
CORPORATE SOURCE: Department of Environmental Sciences, Faculty of Science, Ibaraki University, Mito, 310-8512, Japan
SOURCE: Organic Letters (2003), 5(15), 2679-2681
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:213884

AB In the presence of MS 4Å in DMSO, cyanobenzoylation of various aldehydes RCHO (R = Me3C, Ph, cyclohexyl, n-hexyl, 4-BrC6H4, 2-naphthyl, etc.) with benzoyl cyanide proceeded very smoothly to give the corresponding cyanohydrin benzoates PhCO2CHR(CN) in high to excellent yields (81-97%) without an acid or a base catalyst. On the other hand, reaction of these aldehydes with benzoyl cyanide in DMSO-H2O also occurred readily to afford the corresponding free cyanohydrins RCH(OH)CN exclusively.

IT **53279-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cyanohydrins and cyano esters via hydrocyanation or cyanoacylation of aldehydes with various cyanating reagents)

RN 53279-92-8 CAPLUS
CN Benzenebutanenitrile, α-hydroxy- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
and purified via silica gel column chromatog. to provide hydroxyacetamide IV as colorless powder in 94% yield. Approx. 75 specific examples of I were prepd. The invention is proposed to be useful for the prodn. of statine analogs. The invention process gives products similar to the Passerini reaction, but uses amines instead of isocyanides, and also gives higher yields.

IT **53279-92-8P**
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; preparation of α-hydroxy carbonyl derivs. and related compds. by condensation of carbonyl compds., (silyloxy)propanedinitriles, and amines)

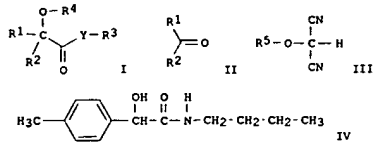
RN 53279-92-8 CAPLUS
CN Benzenebutanenitrile, α-hydroxy- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:444539 CAPLUS
DOCUMENT NUMBER: 137:33079
TITLE: Process for preparation of α-hydroxy amides and related α-hydroxy carbonyl compounds by, e.g., condensation of carbonyl compounds, (silyloxy)propanedinitriles, and amines
INVENTOR(S): Nemoto, Hisao
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: U.S., 34 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6403818	B1	20020611	US 2001-794140	20010228
PRIORITY APPLN. INFO.:			US 2000-185399P P	20000228

OTHER SOURCE(S): CASREACT 137:33079; MARPAT 137:33079
GI



AB A novel process is disclosed for the one-pot preparation of α-hydroxy carbonyl compds. (mostly α-hydroxy amides) of formula I and their derivs. via the condensation of II and III in the presence of R3-YH [wherein: Y = O, S, NR6 (R6 = H, OH, alkyl, alkoxy, cycloalkyl, alkenyl, alkynyl, or (un)substituted 5- to 12-membered heteroaryl group, etc.); R1, R2 independently = H, alkyl, alkoxy, cycloalkyl, bicycloalkyl, alkenyl, alkynyl, heteroaryl or (un)substituted 5- to 12-membered heteroaryl group, etc.; R3 = H, OH, alkyl, alkoxy, cycloalkyl, alkenyl, alkynyl, aryl, (un)substituted 5 to 12-membered heteroaryl group, etc.; R4 = H, substituted silyl protecting group (preferably -SiMe3, -SiMe2tBu or SiPh2tBu), alkanoyl, alkenoyl, alkynoylaryloyl, heteroaryloyl, etc.; R5 = substituted silyl protecting group (preferably -TMS, -TBDMS or -TBDPS), alkanoyl, alkenoyl, alkynoyl, aryloyl, heteroaryloyl, etc.]. A key intermediate in the proposed process is the corresponding acyl cyanide, generated in situ from condensation of II and III. For example, to a stirred solution of 4-methylbenzaldehyde (1.0 mmol) and dinitrile III (R4 = tert-butyldimethylsilyl, 1.2 mmol) in acetonitrile (3 mL) at 0° was added n-butylamine (1.1 mmol) in one portion. After 5 min, a solution of tetrabutylammonium fluoride in THF (1.5 mmol) was added dropwise and the reaction stirred at 0° for an addnl. 20 min. The solution was concentrated

L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:493698 CAPLUS
DOCUMENT NUMBER: 129:135261
TITLE: Enzymic processes for preparing (S)-cyanohydrins
INVENTOR(S): Kirchner, Gerald; Wirth, Irma; Werenka, Christian; Griengl, Herfried; Schmidt, Michael
PATENT ASSIGNEE(S): DSM Chemie Linz G.m.b.H., Austria; Kirchner, Gerald; Wirth, Irma; Werenka, Christian; Griengl, Herfried; Schmidt, Michael
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9830711	A1	19980716	WO 1997-EP2692	19970526
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AT 9700041	A	20000315	AT 1997-41	19970113
AT 406959	B	20001127		
CA 2277916	AA	19980716	CA 1997-2277916	19970526
AU 9731674	A1	19980803	AU 1997-31674	19970526
EP 951561	A1	19991027	EP 1997-927041	19970526
EP 951561	B1	20010808		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
AT 204023	E	20010815	AT 1997-927041	19970526
JP 2001513625	T2	20010904	JP 1998-530486	19970526
ES 2161466	T3	20011201	ES 1997-927041	19970526
US 6337196	B1	20020108	US 1999-331761	19990625
PRIORITY APPLN. INFO.:			AT 1997-41 A	19970113
			WO 1997-EP2692 W	19970526

OTHER SOURCE(S): MARPAT 129:135261

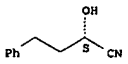
AB The invention concerns an enantioselective process for preparing the (S)-enantiomer of an optically active cyanohydrin by reacting an aldehyde or ketone with a cyanide group donor. According to this process, the aldehyde or ketone is reacted with a cyanide group donor in an organic diluent in the presence of a recombinant (S)-hydroxynitrile lyase from Hevea brasiliensis, the resultant (S)-cyanohydrin being isolated from the reaction mixture

IT **117213-74-8P**, (S)-(-)-2-Hydroxy-4-phenylbutanenitrile
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(enzymic processes for preparing (S)-cyanohydrins)

RN 117213-74-8 CAPLUS
CN Benzenebutanenitrile, α-hydroxy-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L10 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

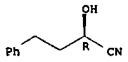
ACCESSION NUMBER: 1994:482105 CAPLUS
DOCUMENT NUMBER: 121:82105
TITLE: Asymmetric carbon-carbon bond forming reactions catalyzed by chiral Schiff base-titanium alkoxide complexes
AUTHOR(S): Hayashi, Masahiko; Inoue, Tetsuya; Miyamoto, Yasunori; Oguni, Nobuki
CORPORATE SOURCE: Fac. Sci., Yamaguchi Univ., Yamaguchi, 753, Japan
SOURCE: Tetrahedron (1994), 50(15), 4385-98
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:82105

AB The enantioselective addition of trimethylsilyl cyanide to a variety of aldehydes proceeded by the aid of a catalyst prepared in situ from titanium tetraisopropoxide and chiral Schiff bases and gave the corresponding cyanohydrins in high optical yield (up to 96% e.e.). A remarkable rate enhancement was brought about by the addition of the Schiff base to the titanium alkoxide mediated silylcyanation of aldehydes. This catalyst system also promoted the highly enantioselective reaction of diketene with aldehydes, which led to the formation of optically active 5-hydroxy-3-oxo **esters**.

IT **120999-41-9P**
RL: PREP (Preparation)
(asym. synthesis of)

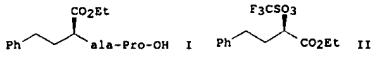
RN 120999-41-9 CAPLUS
CN Benzenebutanenitrile, α-hydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:59951 CAPLUS
DOCUMENT NUMBER: 116:59951
TITLE: Enantioselevtive synthesis of N-[(S)-ethoxycarbonyl-3-phenylpropyl]-L-alanyl-L-proline from chiral synthon prepared enzymatically; a practical method for large-scale synthesis
AUTHOR(S): Tseng, Tsung Chin; Duo, Tsai Hui; Wang, Yi Fong
CORPORATE SOURCE: Sch. Pharm., Kaohsiung Med. Coll., Kaohsiung, 80708, Taiwan
SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (1991), 38(5), 487-90
CODEN: JCCTAC; ISSN: 0009-4536
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:59951
GI

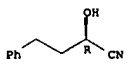


AB The title compound (I) was prepared by treating H-Ala-Pro-OCMe3 with chiral triflate II in the presence of Et3N and de-tert-butylating the resulting product with HCl/dioxane. II was prepared in 4 steps from (R)-PhCH2CH2CH(OH)CN [(R)-III]. (R)-III was prepared by the resolution of (±)-III via lipase-catalyzed acetylation.

IT **120999-41-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and O-tetrahydropyranylation of)

RN 120999-41-9 CAPLUS
CN Benzenebutanenitrile, α-hydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

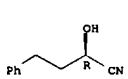
ACCESSION NUMBER: 1991:120946 CAPLUS
DOCUMENT NUMBER: 114:120946
TITLE: Enzyme-catalyzed reactions. 7. Enantioselective esterification of racemic cyanohydrins and enantioselective hydrolysis or transesterification of cyanohydrin **esters** by lipases
AUTHOR(S): Effenberger, Franz; Gutterer, Beate; Ziegler, Thomas; Eckhardt, Elisabeth; Aichholz, Reiner
CORPORATE SOURCE: Inst. Org. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Germany
SOURCE: Liebigs Annalen der Chemie (1991), (1), 47-54
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 114:120946

AB Pure cyanohydrin enantiomers (S)- and (R)-HOCHRCN [R = Pr, Ph, phenethyl, benzo[1,3]dioxol-5-yl, 3,4-MeO(HO)C6H3] and their O-acyl derivs. are obtained from three different lipase-catalyzed reactions: i) enantioselective hydrolysis of aliphatic and aromatic racemic cyanohydrin **esters**, ii) enantioselective acylation of racemic cyanohydrins, and iii) enantioselective transesterification of **esters** with primary alcs. Both the cyanohydrin **esters** and the free cyanohydrins (which are prone to racemization) are isolated as enantiomers with high optical purity on a preparative scale. Hydrolysis of the racemic butyrates with candida cylindracea lipase and pseudomonas sp. lipase, resp., for example, affords (S)-I (R = Pr, Ph) in high yield with 97 and 96% ee, resp. (S)-I (R = Pr) is obtained with the same optical purity by candida sp. lipase-catalyzed transesterification of PrCO2CHPrCN with 1-octanol.

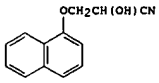
IT **120999-41-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 120999-41-9 CAPLUS
CN Benzenebutanenitrile, α-hydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



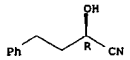
L10 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:594247 CAPLUS
DOCUMENT NUMBER: 111:194247
TITLE: Lipase-catalyzed irreversible transesterification using enol esters: resolution of cyanohydrins and syntheses of ethyl (R)-2-hydroxy-4-phenylbutyrate and (S)-propranolol
AUTHOR(S): Wang, Yi Fong; Chen, Shui Tein; Liu, Kevin K. C.; Wong, Chi Huey
CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SOURCE: Tetrahedron Letters (1989), 30(15), 1917-20
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:194247
GI



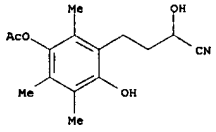
I

AB Racemic hydroxyacetonitriles, (±)-I, (±)-PhCH2CH2CH(OH)CN, and (±)-PhCH2OCH2CH(OH)CN, were resolved by lipoprotein lipase. (±)-I gave (+)-I which was sequentially reduced (LiAlH4) and treated with Me2CO and NaBH4 to give (S)-propranolol.
IT 120999-41-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 120999-41-9 CAPLUS
CN Benzenebutanenitrile, α-hydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



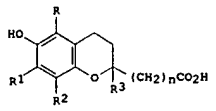
L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:468154 CAPLUS
DOCUMENT NUMBER: 87:68154
TITLE: Antioxidant chroman compounds
INVENTOR(S): Scott, John William; Parrish, David Richard; Saucy, Gabriel
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 30 pp. Division of U.S. 3,947,473.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4018799	A	19770419	US 1975-637611	19751204
US 3947473	A	19760330	US 1973-417465	19731119
CH 622257	A	19810331	CH 1976-14579	19761119
PRIORITY APPLN. INFO.:			US 1972-317566	A2 19721222
			US 1973-417465	A3 19731119
			CH 1973-17771	A 19731219

GI



I

AB Chromanacetic and -carboxylic acids (I; R, R1, R2 = sep. H or alkyl; R3 = H, alkyl, Ph; n = 0 or 1), as racemates or optical anti podes, which showed antioxidant activity by inhibiting development of rancidity in fats and oils and are intermediates for the preparation of α-tocopherol, were prepared by standard methods. Thus, trimethylhydroquinone was treated with HC(OMe)3 and CH2:CHCOMe in the presence of H2SO4, the resultant (±)-2-methoxy-2,5,7,8-tetramethyl-6-chromanol was acetylated, the MeO group hydrolyzed, and treated with (MeO)2PCH2CO2Me and NaH to give the Me ester acetate of I (R = R1 = R2 = R3 = Me, n = 1) (II), which was then converted to II by alkaline hydrolysis. Chicken fat with added II did not become rancid for 16 days, compared to 3 days with no additive.
IT 53713-16-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53713-16-9 CAPLUS
CN Benzenebutanenitrile, 3-(acetyloxy)-α,6-dihydroxy-2,4,5-trimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:505278 CAPLUS
DOCUMENT NUMBER: 81:105278
TITLE: Chromane derivatives
INVENTOR(S): Saucy, Gabriel; Scott, John William; Parrish, David R.
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co., A.-G.
SOURCE: Ger. Offen., 80 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2364141	A1	19740627	DE 1973-2364141	19731221
ZA 7309471	A	19740828	ZA 1973-9471	19731213
CH 603617	A	19780831	CH 1973-17771	19731219
CH 605892	A	19781013	CH 1973-17770	19731219
DD 109624	C	19741112	DD 1973-175557	19731220
BE 808942	A1	19740621	BE 1973-139128	19731221
BE 808943	A1	19740621	BE 1973-139129	19731221
NL 7317587	A	19740625	NL 1973-17587	19731221
NL 7317590	A	19740625	NL 1973-17590	19731221
NL 178968	B	19860116		
NL 178968	C	19860616		
JP 49088876	A2	19740824	JP 1973-142526	19731221
JP 49088877	A2	19740824	JP 1973-142527	19731221
JP 59046233	B4	19841110		
FR 2255299	A1	19750718	FR 1973-46001	19731221
HU 168043	P	19760228	HU 1973-HO1637	19731221
ES 421683	A1	19760401	ES 1973-421683	19731221
FR 2284604	A1	19760409	FR 1973-46000	19731221
FR 2284604	B1	19790511		
AT 7310769	A	19760415	AT 1973-10769	19731221
AT 333755	B	19761210		
SU 518135	D	19760615	SU 1973-1978253	19731221
GB 1456827	A	19761124	GB 1973-59296	19731221
GB 1456828	A	19761124	GB 1973-59298	19731221
GB 1456829	A	19761124	GB 1975-22271	19731221
GB 1456830	A	19761124	GB 1975-22272	19731221
CA 1022562	A1	19771213	CA 1973-188762	19731221
SE 406912	C	19790614	SE 1973-17421	19731221
SE 406912	B	19790305		
AU 7364009	A1	19750703	AU 1973-64009	19731228
CH 622257	A	19810331	CH 1976-14579	19761119
JP 59144780	A2	19840818	JP 1984-5854	19840118
JP 60026795	B4	19850625		
PRIORITY APPLN. INFO.:			US 1972-317566	A 19721222
			CH 1973-17771	A 19731219

GI For diagram(s), see printed CA Issue.
AB Chromancarboxylates such as I (R = H, Me, Et, R1-R3 = Me; R = Me, R1 = H, R2 = R3 = Me, R1 = R2 = CHMe2, R3 = H, R1 = R3 = H, R2 = CMe3) and chromanacetates II (R1 = H, Me) were prepared Thus, trimethylhydroquinone was treated with CH2:CHCOMe and HC(OMe)3 to give 6-hydroxy-2-methoxy-2,5,7,8-tetramethylchroman, which was acetylated, demethylated, and treated with Me3P:CHCO2Me, followed by saponification of the ester group

L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
to give II (R1 = Me), which at 0.02% prevented soybean oil from going rancid in the Schaal oven test at 45° for 12 days, compared with 2 days for the control.

IT 53713-16-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 53713-16-9 CAPLUS

CN Benzenebutanenitrile, 3-(acetyloxy)-α,6-dihydroxy-2,4,5-trimethyl- (9CI) (CA INDEX NAME)